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ERRORS IN FINITE-DIFFERENCE COMPUTATIONS ON CURVILINEAR COORDINATE SYSTEMS

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ERRORS IN FINITE-DIFFERENCE COMPUTATIONS
ON CURVILINEAR COORDINATE SYSTEMS*

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ABSTRACT

Curvilinear coordinate systems have been used extensively to solve partial differential equations on arbitrary regions. An analysis of truncation error in the computation of derivatives reveals why numerical results may be erroneous. A more accurate method of computing derivatives is presented.

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1. Introduction

The use of curvilinear coordinate systems has been a major factor in the solution of many problems by finite difference methods. Some applications in the area of fluid dynamics appear in the papers by Godunov and Prokopov [3], Kutler [5], Steger [7], Steger and Kutler [8] and Thames et. al. [9]. In this report a curvilinear coordinate system is a finite difference mesh with the property that each neighborhood of a mesh point is topologically equivalent to a rectangular mesh in the plane. That is, the coordinate lines can be considered as level curves of some one-to-one transformation. The solution of a partial differential equation can therefore be computed by solving the transformed equation on a rectangular region. The finite difference analog of the transformed equation gives a system of equations which are to be solved to obtain a solution defined on the curvilinear coordinate system (see [9]).

When solving a partial differential equation on an arbitrary two-dimensional region, curvilinear coordinate systems can be constructed so that certain coordinate lines coincide with the boundary contours of the region or move with the boundary in the case of a free boundary problem. By spacing the coordinate lines more closely in regions where there is a rapid change in the solution, the accuracy can often be maintained with fewer mesh points than would be required with a uniform mesh.

There are also difficulties which arise due to the use of a curvilinear coordinate system. The transformed equation will generally be

more complex than the original equation and finite difference methods which can be used to solve the original equation may not be applicable to the transformed equation. Laplace's equation is a classical example where efficient direct methods can be used to solve boundary value problems on rectangular regions. It has also been observed that the coordinate system can have a substantial effect on the error in the numerical solution of a partial differential equation. Evidence of this fact for one-dimensional mesh systems is amply demonstrated by Crowder and Dalton [2] and in a related article by Blottner and Roache [1]. In this report the effect of the coordinate system on error will be analyzed by examining the truncation error in the approximation of partial derivatives by difference expressions on the curvilinear mesh. Our analysis reinforces the view that caution should be used in solving problems on coordinate systems with large curvature, rapidly changing coordinate line spacing, or with coordinate systems which are extremely nonorthogonal. This would be especially true in the case of a singular perturbation problem where the perturbation term might be dominated by the truncation error from other terms.

A method of generating difference expressions is also proposed which incorporates some of the error terms in the traditional method thereby decreasing the truncation error in the derivative approximations. Since error terms are needed, the difference expressions are derived from Taylor series expansions rather than by simpler method of differencing the transformed equations. Standard second order central differences have been used throughout so that an error analysis or an improved difference formulation could be inserted into an existing computer program with a minimum of modification to the code. Although

only quadrilateral meshes are considered in this report, a similar analysis could be carried out for difference formulations on triangular meshes used by Winslow [10] and others. Related results for one-dimensional finite difference meshes are contained in the paper by Kelney de Rivas [4] and the book by Roache [6].

2. Difference Equations on a Curvilinear Coordinate System

Suppose that a curvilinear coordinate system is given in a region R of the xy -plane. Let f be a function in $C^3(R)$. Difference expressions for the first and second order partial derivatives of f can be obtained by transforming the curvilinear mesh to a rectangular mesh and applying the chain rule. The derivatives of f in terms of the transformed $\xi\eta$ -variables are related to the derivatives in the xy -plane by the following equations.

$$\begin{aligned}\frac{\partial f}{\partial \xi} &= \frac{\partial x}{\partial \xi} \frac{\partial f}{\partial x} + \frac{\partial y}{\partial \xi} \frac{\partial f}{\partial y}, & \frac{\partial f}{\partial \eta} &= \frac{\partial x}{\partial \eta} \frac{\partial f}{\partial x} + \frac{\partial y}{\partial \eta} \frac{\partial f}{\partial y} \\ \frac{\partial^2 f}{\partial \xi^2} &= \frac{\partial^2 x}{\partial \xi^2} \frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \xi^2} \frac{\partial f}{\partial y} + \left(\frac{\partial x}{\partial \xi}\right)^2 \frac{\partial^2 f}{\partial x^2} + 2 \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} \frac{\partial^2 f}{\partial x \partial y} + \left(\frac{\partial y}{\partial \xi}\right)^2 \frac{\partial^2 f}{\partial y^2} \\ \frac{\partial^2 f}{\partial \xi \partial \eta} &= \frac{\partial^2 x}{\partial \xi \partial \eta} \frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \xi \partial \eta} \frac{\partial f}{\partial y} + \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} \frac{\partial^2 f}{\partial x^2} + \left(\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi}\right) \frac{\partial^2 f}{\partial x \partial y} + \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} \frac{\partial^2 f}{\partial y^2} \\ \frac{\partial^2 f}{\partial \eta^2} &= \frac{\partial^2 x}{\partial \eta^2} \frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \eta^2} \frac{\partial f}{\partial y} + \left(\frac{\partial x}{\partial \eta}\right)^2 \frac{\partial^2 f}{\partial x^2} + 2 \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \eta} \frac{\partial^2 f}{\partial x \partial y} + \left(\frac{\partial y}{\partial \eta}\right)^2 \frac{\partial^2 f}{\partial y^2}\end{aligned} \quad (1)$$

The derivatives with respect to the xy -variables can be expressed in terms of derivatives with respect to $\xi\eta$ -variables provided the Jacobian of the transformation does not vanish. Now consider a mesh point P with neighbors as indicated in Figure 1. All derivatives with respect to $\xi\eta$ -variables can be approximated using classical difference operators. Thus we define the following expressions which replace the corresponding derivatives in (1).

$$\begin{aligned}
f_{\xi}(P) &= (f(Q) - f(R))/2 \\
f_{\eta}(P) &= (f(S) - f(T))/2 \\
f_{\xi\xi}(P) &= f(Q) + f(R) - 2f(P) \\
f_{\xi\eta}(P) &= (f(U) - f(V) + f(W) - f(X))/4 \\
f_{\eta\eta}(P) &= f(S) + f(T) - 2f(P)
\end{aligned} \tag{2}$$

Of course these are simply the second order central differences on a square mesh of unit width in the $\xi\eta$ -plane. Note that the coordinates x and y are also functions defined on the mesh and their derivatives in (1) can also be approximated by difference expressions. In this manner the system of equations (1) gives rise to difference approximations for the derivatives of f at any mesh point P . These approximations can be used to obtain a finite difference analog of any first or second order partial differential equation. Unfortunately, this method gives no information on the accuracy of the difference approximation.

3. Truncation Error

For a given curvilinear coordinate system defined in a neighborhood of P , we will associate a parameter h which will be a measure of the fineness of the mesh. It will be sufficient for our purposes to assume that the distance between any two adjacent mesh points is bounded above by a constant multiple of h . Thus, when f is x or y , all the difference expressions in (2) must be of order h , at least.

A Taylor series expansion of the function f about the point P yields the following relations between the partial derivatives of f and the difference expressions in (2).

$$\begin{aligned}
f_{\xi} &= x_{\xi} \frac{\partial f}{\partial x} + y_{\xi} \frac{\partial f}{\partial y} + \frac{1}{2} x_{\xi} x_{\xi\xi} \frac{\partial^2 f}{\partial x^2} + \frac{1}{2} (x_{\xi} y_{\xi\xi} + y_{\xi} x_{\xi\xi}) \frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2} y_{\xi} y_{\xi\xi} \frac{\partial^2 f}{\partial y^2} + \epsilon_1 \\
f_{\eta} &= x_{\eta} \frac{\partial f}{\partial x} + y_{\eta} \frac{\partial f}{\partial y} + \frac{1}{2} x_{\eta} x_{\eta\eta} \frac{\partial^2 f}{\partial x^2} + \frac{1}{2} (x_{\eta} y_{\eta\eta} + y_{\eta} x_{\eta\eta}) \frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2} y_{\eta} y_{\eta\eta} \frac{\partial^2 f}{\partial y^2} + \epsilon_2 \\
f_{\xi\xi} &= x_{\xi\xi} \frac{\partial f}{\partial x} + y_{\xi\xi} \frac{\partial f}{\partial y} + \left(\frac{1}{4} x_{\xi\xi}^2 + x_{\xi}^2 \right) \frac{\partial^2 f}{\partial x^2} + \left(\frac{1}{2} x_{\xi\xi} y_{\xi\xi} + 2x_{\xi} y_{\xi} \right) \frac{\partial^2 f}{\partial x \partial y} \\
&\quad + \left(\frac{1}{4} y_{\xi\xi}^2 + y_{\xi}^2 \right) \frac{\partial^2 f}{\partial y^2} + \epsilon_{11} \\
f_{\xi\eta} &= x_{\xi\eta} \frac{\partial f}{\partial x} + y_{\xi\eta} \frac{\partial f}{\partial y} + \frac{1}{2} ((x^2)_{\xi\eta} - 2x x_{\xi\eta}) \frac{\partial^2 f}{\partial x^2} + ((xy)_{\xi\eta} - x y_{\xi\eta} - y x_{\xi\eta}) \frac{\partial^2 f}{\partial x \partial y} \\
&\quad + \frac{1}{2} ((y^2)_{\xi\eta} - 2y y_{\xi\eta}) \frac{\partial^2 f}{\partial y^2} + \epsilon_{12} \\
f_{\eta\eta} &= x_{\eta\eta} \frac{\partial f}{\partial x} + y_{\eta\eta} \frac{\partial f}{\partial y} + \left(\frac{1}{4} x_{\eta\eta}^2 + x_{\eta}^2 \right) \frac{\partial^2 f}{\partial x^2} + \left(\frac{1}{2} x_{\eta\eta} y_{\eta\eta} + 2x_{\eta} y_{\eta} \right) \frac{\partial^2 f}{\partial x \partial y} \\
&\quad + \left(\frac{1}{4} y_{\eta\eta}^2 + y_{\eta}^2 \right) \frac{\partial^2 f}{\partial y^2} + \epsilon_{22}
\end{aligned} \tag{3}$$

All remainder terms are $O(h^3)$. In the first two equations of (3), if only the first order terms are retained, the remainder terms, say ϵ_1' and ϵ_2' , would be $O(h^2)$. In this case we would have

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{1}{J} (f_{\xi} y_{\eta} - f_{\eta} y_{\xi}) - \frac{1}{J} (\epsilon_1' y_{\eta} - \epsilon_2' y_{\xi}) \\
\frac{\partial f}{\partial y} &= \frac{1}{J} (f_{\eta} x_{\xi} - f_{\xi} x_{\eta}) - \frac{1}{J} (\epsilon_2' x_{\xi} - \epsilon_1' x_{\eta})
\end{aligned} \tag{4}$$

where

$$J = x_{\xi} y_{\eta} - x_{\eta} y_{\xi}.$$

The first terms on the right of (4) are the same difference approximations for the first order partial derivatives as would be obtained by differencing the first two equations of (1). Consequently, the truncation error in the finite difference expressions for the first partial derivatives of f from the transformation method would be $O(h)$ provided

$$\left| \frac{\epsilon_1}{J} \right|, \left| \frac{\epsilon_2}{J} \right| = O(1)$$

or simply

$$\left| \frac{h^2}{J} \right| = O(1).$$

Now comparing the last three equations in (1) and (3), we see that the difference expressions for the second order derivatives from (1) would derive from the following equations which include a truncation term.

$$\begin{aligned} x_\xi^2 \frac{\partial^2 f}{\partial x^2} + 2x_\xi y_\xi \frac{\partial^2 f}{\partial x \partial y} + y_\xi^2 \frac{\partial^2 f}{\partial y^2} &= f_{\xi\xi} - \frac{1}{J}(x_{\xi\xi}y_\eta - y_{\xi\xi}x_\eta)f_\xi \\ &\quad - \frac{1}{J}(y_{\xi\xi}x_\xi - x_{\xi\xi}y_\xi)f_\eta + \epsilon_{11} \\ x_\xi x_\eta \frac{\partial^2 f}{\partial x^2} + (x_\xi y_\eta + x_\eta y_\xi) \frac{\partial^2 f}{\partial x \partial y} + y_\xi y_\eta \frac{\partial^2 f}{\partial y^2} &= f_{\xi\eta} - \frac{1}{J}(x_{\xi\eta}y_\eta - y_{\xi\eta}x_\eta)f_\xi \\ &\quad - \frac{1}{J}(y_{\xi\eta}x_\xi - x_{\xi\eta}y_\xi)f_\eta + \epsilon_{12} \\ x_\eta^2 \frac{\partial^2 f}{\partial x^2} + 2x_\eta y_\eta \frac{\partial^2 f}{\partial x \partial y} + y_\eta^2 \frac{\partial^2 f}{\partial y^2} &= f_{\eta\eta} - \frac{1}{J}(x_{\eta\eta}y_\eta - y_{\eta\eta}x_\eta)f_\xi \\ &\quad - \frac{1}{J}(y_{\eta\eta}x_\xi - x_{\eta\eta}y_\xi)f_\eta + \epsilon_{22} \end{aligned} \quad (5)$$

Comparing (5) with (3) we note that the terms ϵ_{11}' , ϵ_{12}' , and ϵ_{22}' would be $O(h^2)$ since some second order terms in (3) would have to be combined with the remainder terms to reproduce the equations in (5). The determinant of the coefficient matrix is J^3 and therefore the truncation error in the second derivative approximation is only $O(1)$ provided

$$\left| \frac{h^2}{J} \right| = O(1).$$

Our remarks should not lead one to conclude that the equations (1) cannot be used to formulate accurate difference equations. The equations obtained by this change of variable technique have been used extensively to solve many problems on curvilinear coordinate systems. It can be said that care should be used in selecting the coordinate system. For example, if

$$|x_{\xi\xi}|, |x_{\eta\eta}|, |y_{\xi\xi}|, |y_{\eta\eta}| = O(h^2),$$

then the truncation errors in the first derivative approximations in (4) are $O(h^2)$. No simple relation between the coefficients in the equation for $f_{\xi\eta}$ in (3) and (5) was found except for the fact that they would be equal if the differences were replaced by derivatives. Hence no general conclusions are drawn on the second derivative approximations. In the special case where the transformation is given by equations of the type

$$x = \phi(\xi), y = \psi(\eta),$$

then the above condition on the second order differences of the coordinate functions implies that the truncation errors for $\partial^2 f / \partial x^2$ and $\partial^2 f / \partial y^2$ from (5) are $O(h)$.

Geometrically, the requirement that the second order differences of x and y be small means that the point P in Figure 1 and the midpoints of the line segments QR and ST should all be close together. This effectively limits the rate of change in coordinate line spacing and the curvature of the coordinate lines. Even for the above error estimates, it was necessary to impose limits on the quantity J . Small values of J also produce larger truncation errors due to the factor $1/J$ in (4) and a $1/J^3$ factor which would appear in solving the system (5). Thus we see why extremely nonorthogonal coordinate systems sometimes give poor numerical results.

4. Increasing Accuracy in Difference Equations

For a general curvilinear coordinate system, more accurate difference approximations for the partial derivatives of f can be obtained by using all first and second order terms of (3). If the system (3) is written in matrix form as

$$\Delta = AD + E,$$

where E contains the remainder term, then the derivatives are given by

$$D = A^{-1}\Delta - A^{-1}E.$$

We will assume that

$$\left| \frac{h^8}{\det(A)} \right| = O(1)$$

which is analogous to the previous condition on J . Since all components of E are $O(h^3)$, the first two columns of A are $O(h)$ and the last three columns of A are $O(h^2)$, it is easily shown that the first two components

of $A^{-1}E$ are $O(h^2)$ while the last three are $O(h)$. Thus $A^{-1}\Delta$ contains difference expressions with a truncation error of $O(h^2)$ for the first order partial derivatives of f and a truncation error of $O(h)$ for the second order partial derivatives of f .

It is difficult to determine the geometric meaning of the condition on $\det(A)$. We do observe a few cases when $\det(A) = 0$, however, they could not occur under our definition of a curvilinear coordinate system. For example, if all points of Figure 1 were colinear or if P coincided with Q , R , S , or T , then $\det(A) = 0$. This observation suggests that erroneous results could occur with coordinate systems having a value of $\det(A)$ which is too small.

For many problems, the cost in computer time and storage of using the difference formulations of (3) rather than (4) and (5) would be very little. A total of 25 coefficients would be needed at each mesh point to compute all first and second order derivatives rather than 19 in the latter case. The inversion of the fifth order matrix A at each mesh point would not be prohibitive unless the inverse had to be recomputed frequently. This would be the case if the curvilinear coordinate system moved during the solution of the problem as might be the case in solving a free boundary problem.

5. Examples

We now look at a couple of coordinate systems and emphasize some of the analysis that might be used to determine the appropriate method of generating difference equations. Let R be the square region given by $0 \leq x, y \leq 1$. The coordinate lines will be parallel to the x and y axes and are given by the equations

$$x = (e^{\frac{n}{N}} - 1)/(e - 1), \quad n = 0, 1, \dots, N,$$

$$y = (e^{\frac{m}{M}} - 1)/(e - 1), m = 0, 1, \dots, M.$$

Computing the nonzero differences of x , say x_ξ and $x_{\xi\xi}$, we have the following approximations for large N .

$$x_\xi \approx \frac{2}{N(e - 1)} e^{\frac{n}{N}}$$

$$x_{\xi\xi} \approx \frac{1}{N^2(e - 1)} e^{\frac{n}{N}}$$

Similar approximations hold for the differences of y . In this example we see that, for large values of M and N , the first order differences are much larger than the second order differences. If h is taken to be the minimal spacing between coordinate lines, then $x_\xi \leq 2eh$ whereas $x_{\xi\xi} \leq e(e - 1)h^2$. Also note that $J \geq 4h^2$. A straightforward differencing of the transformed equations using (4) and (5) would produce difference approximations which are second order accurate for a first order partial derivative and first order accurate for a second order partial derivative. This is true even for the mixed derivative since $(xy)_{\xi\eta} = x_\xi y_\eta$ and $(x^2)_{\xi\eta} = (y^2)_{\xi\eta} = 0$.

Now a coordinate system will be defined on the same region R , but approximation of derivatives by (4) and (5) would not be advisable due to the rapid change in coordinate line spacing. Suppose the coordinate lines are given by

$$x = (e^n - 1)/(e^N - 1), n = 0, 1, \dots, N,$$

$$y = (e^m - 1)/(e^M - 1), m = 0, 1, \dots, M.$$

Then

$$x_{\xi} \approx \frac{1.18}{e^N - 1} e^n$$

$$x_{\xi\xi} \approx \frac{1.08}{e^N - 1} e^n$$

with similar expressions for y . In this example, the difference expressions for second derivatives using (5) would have a truncation error with terms which are nearly one forth as large as terms used in the difference formulation. Thus all first and second order terms in the series expansions (3) would be needed for accurate difference approximations of the derivatives of the function f . For rectangular coordinate systems, the determinant of the coefficient matrix A can be easily computed.

$$\begin{aligned} \det(A) &= (x_{\xi} y_{\eta})^2 (y_{\eta}^2 - \frac{1}{4} y_{\eta\eta}^2) (x_{\xi}^2 - \frac{1}{4} x_{\xi\xi}^2) \\ &\geq \frac{9}{16} x_{\xi\xi}^4 y_{\eta\eta}^4 \\ &\geq \frac{9}{16} h^8 \end{aligned}$$

The parameter h could be viewed as the local minimal coordinate line spacing due to the large variation in coordinate line spacing throughout the region R . The above lower bound on $\det(A)$ is sufficient to guarantee that the approximation of derivatives by (3) would result in $O(h^2)$ and $O(h)$ truncation errors for derivatives of first and second order, respectively.

6. Analytic Transformations

The analysis so far has assumed that all derivatives in the $\xi\eta$ -variables are approximated by differences. If the coordinate system is generated by a simple continuous mapping function, as in the above example, then the derivatives of x and y can be computed and used in transformation equations (1). A similar error analysis can be performed for the difference equations derived from this type of analytic transformation method. The previous method of generating difference equations will be referred to as a numerical transformation method since only the coordinates of the grid points are required.

Due to the similarity in the series expansions for the analytic and numerical transformations, a detailed analysis of truncation error will not be included. It is clear from the following approximation formulas that the order of accuracy would depend on the orders of magnitude of all derivatives of x and y with respect to ξ and η .

For the first order central differences in the computational region, we will assume that f , as a function of ξ and η , is sufficiently smooth so that

$$f_{\xi} \approx \frac{\partial f}{\partial \xi} + \frac{1}{6} \frac{\partial^3 f}{\partial \xi^3} . \quad (6)$$

The right hand sides will now be replaced by derivatives with respect to the physical variables. In order to have a comparison with numerical transformations, only the first and second order derivatives are retained.

$$\begin{aligned} f_{\xi} \approx & \left(\frac{\partial x}{\partial \xi} + \frac{1}{6} \frac{\partial^3 x}{\partial \xi^3} \right) \frac{\partial f}{\partial x} + \left(\frac{\partial y}{\partial \xi} + \frac{1}{6} \frac{\partial^3 y}{\partial \xi^3} \right) \frac{\partial f}{\partial y} + \frac{1}{2} \frac{\partial x}{\partial \xi} \frac{\partial^2 x}{\partial \xi^2} \frac{\partial^2 f}{\partial x^2} \\ & + \frac{1}{2} \left(\frac{\partial x}{\partial \xi} \frac{\partial^2 y}{\partial \xi^2} + \frac{\partial^2 x}{\partial \xi^2} \frac{\partial y}{\partial \xi} \right) \frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2} \frac{\partial y}{\partial \xi} \frac{\partial^2 y}{\partial \xi^2} \frac{\partial^2 f}{\partial y^2} \end{aligned}$$

The inclusion of additional terms in (6) would introduce additional higher order terms in the coefficients of the derivatives of f . Approximations for the second order differences are derived in a similar fashion. If the assumption is made that

$$f_{\xi\xi} = \frac{\partial^2 f}{\partial \xi^2} + \frac{1}{12} \frac{\partial^4 f}{\partial \xi^4} \quad \text{and} \quad f_{\xi\eta} = \frac{\partial^2 f}{\partial \xi \partial \eta} - \frac{1}{6} \left(\frac{\partial^4 f}{\partial \xi^3 \partial \eta} + \frac{\partial^4 f}{\partial \xi \partial \eta^3} \right)$$

then the following estimates hold after dropping all but the first and second order terms.

$$\begin{aligned} f_{\xi\xi} = & \left(\frac{\partial^2 x}{\partial \xi^2} + \frac{1}{12} \frac{\partial^4 x}{\partial \xi^4} \right) \frac{\partial f}{\partial x} + \left(\frac{\partial^2 y}{\partial \xi^2} + \frac{1}{12} \frac{\partial^4 y}{\partial \xi^4} \right) \frac{\partial f}{\partial y} + \left[\left(\frac{\partial x}{\partial \xi} \right)^2 + \frac{1}{4} \left(\frac{\partial^2 x}{\partial \xi^2} \right)^2 \right. \\ & + \frac{1}{3} \frac{\partial x}{\partial \xi} \frac{\partial^3 x}{\partial \xi^3} \left. \right] \frac{\partial^2 f}{\partial x^2} + \left(2 \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} + \frac{1}{2} \frac{\partial^2 x}{\partial \xi^2} \frac{\partial^2 y}{\partial \xi^2} + \frac{1}{3} \frac{\partial x}{\partial \xi} \frac{\partial^3 y}{\partial \xi^3} \right. \\ & + \left. \frac{1}{3} \frac{\partial^3 x}{\partial \xi^3} \frac{\partial y}{\partial \xi} \right) \frac{\partial^2 f}{\partial x \partial y} + \left[\left(\frac{\partial y}{\partial \xi} \right)^2 + \frac{1}{4} \left(\frac{\partial^2 y}{\partial \xi^2} \right)^2 + \frac{1}{3} \frac{\partial y}{\partial \xi} \frac{\partial^3 y}{\partial \xi^3} \right] \frac{\partial^2 f}{\partial y^2} \\ f_{\xi\eta} = & \left[\frac{\partial^2 x}{\partial \xi \partial \eta} - \frac{1}{6} \left(\frac{\partial^4 x}{\partial \xi^3 \partial \eta} + \frac{\partial^4 x}{\partial \xi \partial \eta^3} \right) \right] \frac{\partial f}{\partial x} + \left[\frac{\partial^2 y}{\partial \xi \partial \eta} - \frac{1}{6} \left(\frac{\partial^4 y}{\partial \xi^3 \partial \eta} \right. \right. \\ & + \left. \left. \frac{\partial^4 y}{\partial \xi \partial \eta^3} \right) \right] \frac{\partial f}{\partial y} + \left[\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{1}{6} \left(\frac{\partial^3 x}{\partial \xi^3} \frac{\partial x}{\partial \eta} + \frac{\partial x}{\partial \xi} \frac{\partial^3 x}{\partial \eta^3} \right) - \frac{1}{2} \left(\frac{\partial x}{\partial \xi} \frac{\partial^3 x}{\partial \xi^2 \partial \eta} \right. \right. \\ & + \left. \frac{\partial x}{\partial \eta} \frac{\partial^3 x}{\partial \xi \partial \eta^2} + \frac{\partial^2 x}{\partial \xi^2} \frac{\partial^2 x}{\partial \xi \partial \eta} + \frac{\partial^2 x}{\partial \xi \partial \eta} \frac{\partial^2 x}{\partial \eta^2} \right] \frac{\partial^2 f}{\partial x^2} + \left[\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} \right. \\ & - \frac{1}{6} \left(\frac{\partial x}{\partial \xi} \frac{\partial^3 y}{\partial \eta^3} + \frac{\partial^3 x}{\partial \xi^3} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial^3 y}{\partial \xi^3} + \frac{\partial^3 x}{\partial \xi^3} \frac{\partial y}{\partial \xi} \right) - \frac{1}{2} \left(\frac{\partial x}{\partial \xi} \frac{\partial^3 y}{\partial \xi^2 \partial \eta} \right. \\ & + \left. \frac{\partial x}{\partial \eta} \frac{\partial^3 y}{\partial \xi \partial \eta^2} + \frac{\partial^3 x}{\partial \xi^2 \partial \eta} \frac{\partial y}{\partial \xi} + \frac{\partial^3 x}{\partial \xi \partial \eta^2} \frac{\partial y}{\partial \eta} + \frac{\partial^2 x}{\partial \xi \partial \eta} \left(\frac{\partial^2 y}{\partial \xi^2} + \frac{\partial^2 y}{\partial \eta^2} \right) \right] \frac{\partial^2 f}{\partial x \partial y} \end{aligned}$$

$$\begin{aligned}
& + \frac{\partial^2 y}{\partial \xi \partial \eta} \left(\frac{\partial^2 x}{\partial \xi^2} + \frac{\partial^2 x}{\partial \eta^2} \right) \Big] \frac{\partial^2 f}{\partial x \partial y} + \left[\frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{1}{6} \left(\frac{\partial y}{\partial \xi} \frac{\partial^3 y}{\partial \eta^3} + \frac{\partial^3 y}{\partial \xi^3} \frac{\partial y}{\partial \eta} \right) \right. \\
& \left. - \frac{1}{2} \left(\frac{\partial y}{\partial \xi} \frac{\partial^3 y}{\partial \xi^2 \partial \eta} + \frac{\partial y}{\partial \eta} \frac{\partial^3 y}{\partial \xi \partial \eta^2} + \frac{\partial^2 y}{\partial \xi^2} \frac{\partial^2 y}{\partial \xi \partial \eta} + \frac{\partial^2 y}{\partial \xi \partial \eta} \frac{\partial^2 y}{\partial \eta^2} \right) \right] \frac{\partial^2 f}{\partial y^2} .
\end{aligned}$$

Again we observe that the traditional difference formulations for the derivatives of f are accurate only if the higher order derivatives of the coordinate functions x and y become progressively smaller.

In the above error analysis for both numerical and analytic transformations, it was assumed that certain remainder terms in the Taylor series expansions were negligible. This implies the third order derivatives of f with respect to the physical variables must be bounded and these bounds depend on the coordinate line spacing. A comparison of the above approximations also suggest that the numerical computation of the derivative coefficients would be preferred due to the appearance of error in the first derivative terms when the coefficients are computed analytically. On the other hand, for the numerical transformation, the coefficients of the second derivative terms in the expression for $\frac{\partial^2 f}{\partial \xi \partial \eta}$ appear to have little relation to the coefficients encountered in the usual change of variables formulation. The differential analogs of the corresponding difference expressions for the coefficients would, however, be equal.

Equivalent estimates would hold for central differences for functions of three variables. These expressions are omitted since they are even more length than those given above.

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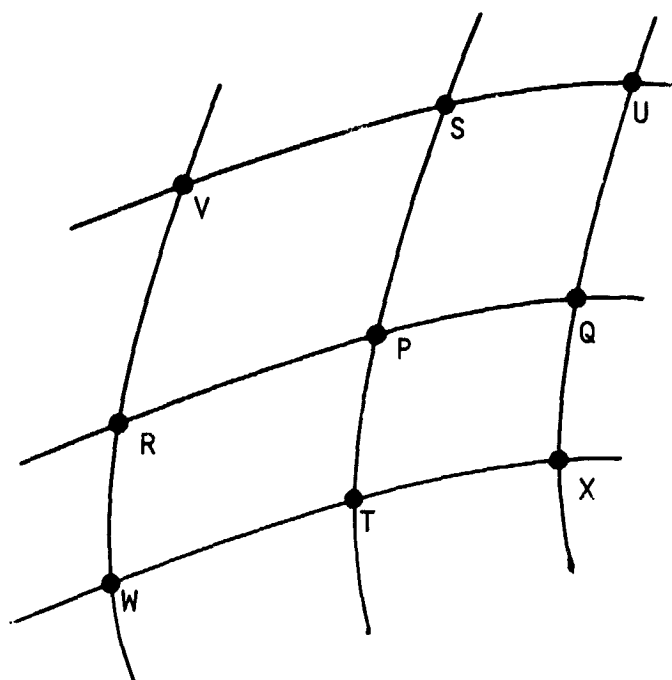


Figure 1. Computational molecule